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# Numerical analysis of surface plasmons excited on a thin metal grating<sup>\*</sup>

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**Abstract:** The authors numerically investigated the characteristics of surface plasmons excited on a thin metal grating placed in planer or conical mounting. After formulating the problem, the solution method, Yasuura's method (a modal expansion approach with least-squares boundary matching) was described. Although the grating is periodic in one direction, coupling between TE and TM waves occurs because arbitrary incidence is assumed. This requires the employment of both TE and TM vector modal functions in the analysis. Numerical computations showed: (1) the excitation of surface plasmons with total or partial absorption of incident light; (2) the resonance character of the coefficient of an evanescent order that couples the plasmon surface wave; (3) the field profile and Poynting's vector. The plasmons excited on the surfaces of a thin metal grating are classified into three types: SISP, SRSP, and LRSP, different from each other in the feature of field profile and energy flow. In addition, the eigenvalue of a plasmon mode was obtained by solving a sequence of diffraction problems with complex-valued angles of incidence and using the quasi-Newton algorithm to predict the real angle of incidence at which the absorption occurs.

Key words:Thin metal grating, Plasmon modes, Resonance absorption, Numerical analysisdoi:10.1631/jzus.2006.A0055Document code: ACLC number: 0441

# INTRODUCTION

It is widely known that a metal grating supports plasmon surface waves in the optics region (Raeter, 1982; Nevier, 1980). Excitation of a plasmon surface wave causes resonance absorption, which can be observed as partial or total absorption of incident light accompanied by an abrupt change of diffraction efficiency called resonance anomaly.

If the grating is thick enough, the surface waves can be excited on the lit surface alone and the surface waves in this case are called single-interface surface plasmon (SISP). While if the grating is thin, which is the case we are interested in, simultaneous excitation of plasmon surface waves on both the surfaces occurs. The plasmons interact with each other to form two types of coupled plasmon modes: a short-range surface plasmon (SRSP) and a long-range surface plasmon (LRSP).

When a thin metal grating is illuminated by a monochromatic plane wave, resonance absorption occurs at the angles of incidence at which the SRSP and LRSP are excited. The angles are called resonance angles and are determined by the phasematching condition: The phase constant of an evanescent order agrees with the real part of an eigenvalue of a plasmon mode. Because the coupled modes are different in eigenvalues, two absorption dips corresponding to two coupled modes are observed.

In the following sections we first formulate the problem of diffraction by a thin metal grating assuming that the grating is placed in conical mounting. That is, the plane of incidence spanned by the incident wavevector and the grating normal is assumed to

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make an arbitrary azimuth angle with the direction of periodicity. If the azimuth is zero, the placement is termed planer or classical mounting. In a planer mounting case the resonance absorption can be seen for TM-wave (*p* polarization) incidence alone. While in a conical mounting case, it is observed for both TE-wave (*s* polarization) and TM-wave incidence.

After describing the problem, we introduce briefly the solution method: Yasuura's method (Yasuura and Itakura, 1965; 1966a; 1966b; Yasuura, 1971; Okuno, 1990). It is a modal expansion approach combined with least-squares boundary matching. Approximate solutions inside and outside of the metal layer are defined in terms of linear combinations of vector modal functions with unknown coefficients. The coefficients are determined in order that the solutions satisfy the boundary conditions in the leastsquares sense.

On the other hand, by solving a sequence of diffraction problems with complex-valued incident angles and using the quasi-Newton iteration algorithm, we can find the eigenvalues of the plasmon modes. Having the eigenvalues of a grating, we can predict the resonance angles by applying the phase-matching condition.

Numerical computations were carried out for a relatively thick (the thickness to period ratio is 0.4 and the period is a little less than the wavelength) and two thin gratings (the ratio is 0.08 or 0.02). After observing the resonance absorption as dips in efficiency curves, we show the resonant character of the modal coefficient of an evanescent order, the field distribution, and energy flow. Besides, we illustrate the thickness dependence of the eigenvalues obtained by the iteration procedure. Prediction of the resonance angles from the eigenvalues agrees well with the numerical result for the diffraction problems.

## FORMULATION OF THE PROBLEM

Fig.1 illustrates the schematic representation of diffraction by a thin metal grating. The grating is uniform in y and is corrugated in x with a period d. The grating has an upper and a lower surface, which are given by

$$\begin{cases} S_1: \ z_1 = \eta_1(x) = h \sin(2\pi x/d), \\ S_2: \ z_2 = \eta_2(x) = \eta_1(x) - e, \end{cases}$$
(1)



Fig.1 Schematic representation of diffraction by a thin metal grating. (a) Conical mounting; (b) Planer mounting

where *e* and *h* are thickness and amplitude of the grating. Note that (x,z) denotes a point on the surface of the grating while P=(X,Z) denotes a point inside a region. The surfaces separate the whole space into three regions:  $V_1[Z > \eta_1(X)]$ ,  $V_2[\eta_1(X) > Z > \eta_2(X)]$ , and  $V_3[Z < \eta_1(X)]$ . We assume that the region  $V_2$  is occupied by a metal with a complex-valued refractive index  $n_2$  and that regions  $V_1$  and  $V_3$  are vacuums  $(n_1=n_3=1)$ .

The electric and magnetic field of an incident light are given by

$$\begin{bmatrix} \boldsymbol{E}^{i} \\ \boldsymbol{H}^{i} \end{bmatrix} (\boldsymbol{P}) = \begin{bmatrix} \boldsymbol{e}^{i} \\ \boldsymbol{h}^{i} \end{bmatrix} \exp(j\boldsymbol{k}^{i} \cdot \boldsymbol{P} - j\omega t), \quad (2)$$

and

$$\boldsymbol{h}^{i} = (1/\omega\mu_{0})\boldsymbol{k}^{i} \times \boldsymbol{e}^{i}, \qquad (3)$$

here,  $e^{i}$  is the electric field amplitude,  $h^{i}$  is the magnetic field amplitude and  $k^{i}$  is the incident wavevector

defined by

$$\boldsymbol{k}^{i} = (\alpha, \beta, -\gamma), \qquad (4)$$

where  $\alpha = n_1 \mathbf{k} \sin \theta \cos \phi$ ,  $\beta = n_1 \mathbf{k} \sin \theta \sin \phi$ ,  $\gamma = n_1 \mathbf{k} \cos \theta$ , and  $\mathbf{k} = 2\pi/\lambda$ .

As shown in Fig.1a,  $\theta$  is the polar angle between the z axis and the incident wavevector  $k^i$ , and  $\phi$  is the azimuth angle between the x axis and the plane of incidence. When  $\phi=0$  in Fig.1a, the incident light comes from a direction orthogonal to the grooves as shown in Fig.1b. This arrangement is called planer or classical mounting, in which the diffracted waves propagate in directions in the plane of incidence. While if  $\phi\neq0$  as in Fig.1a, the directions in which the diffracted waves travel lie on a cone centered at the origin. This is termed conical mounting. Because the planer mounting is a special case, we confine ourselves to the conical mounting case in the following discussion.

Let us decompose the electric amplitude  $e^i$  of the incident light into a transverse-electric (TE) and a transverse-magnetic (TM) component. Here, the TE or TM means the absence of the *z*-component in the relevant electric or magnetic field. To do this we first define two unit vectors that span a plane orthogonal to  $k^i$  taking into account that  $e^i$  is on that plane:

$$\begin{cases} \boldsymbol{e}^{\mathrm{TE}} = (\sin\phi, -\cos\phi, 0), \\ \boldsymbol{e}^{\mathrm{TM}} = (\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta). \end{cases}$$
(5)

Apparently,  $e^{\text{TE}}$  has no *z* component. The fact that the magnetic field accompanying  $e^{\text{TM}}$  cannot have any *z* component is seen by direct manipulation. In addition, they are perpendicular to each other and both of them make a right angle with  $k^i$ . Hence,  $e^{\text{TE}}$  and  $e^{\text{TM}}$  are the unit vectors in the directions of the TE and TM component in the sense above. The electric field amplitude  $e^i$  is decomposed as

$$\boldsymbol{e}^{\mathrm{i}} = \boldsymbol{e}^{\mathrm{TE}} \cos \delta + \boldsymbol{e}^{\mathrm{TM}} \sin \delta, \qquad (6)$$

where  $\delta$  is the angle between  $e^{\text{TE}}$  and  $e^{i}$  (Fig.2) and is termed a polarization angle. In particular,  $\delta=0$  and  $\delta=\pi/2$  stand for TE (or *s*) and TM (or *p*) wave incidence. Thus, the incident light is specified by a wavelength  $\lambda$ , an azimuth angle  $\phi$ , a polar angle  $\theta$ , and a polarization angle  $\delta$ . The time factor  $e^{-j\omega t}$  will be suppressed hereafter.



Fig.2 Definition of a polarization angle

We denote by  $E_j^d(P)$  and  $H_j^d(P)$  the diffracted electric and magnetic field in  $V_j$  (*j*=1, 2, 3). They satisfy the following requirements:

(D1) Helmholtz's equations in each region;

(D2) A periodicity condition that  $f(X+d,Z)=e^{j\alpha d}f(X,Z)$ , where *f* denotes any component of  $E_{j}^{d}(P)$  or  $H_{j}^{d}(P)$ ;

(D3) A radiation condition in z that the diffracted field in  $V_1$  (or in  $V_3$ ) propagates or attenuates in the positive (or negative) z direction;

(D4) The boundary conditions that the tangential components of the total electric and magnetic fields are continuous across the boundaries  $S_1$  and  $S_2$ .

## METHOD OF SOLUTION

We employ Yasuura's method (Yasuura and Itakura, 1965a; 1996a; 1966b; Yasuura, 1971; Okuno, 1990) in solving the problem above on a computer, the method which is a modal expansion approach combined with least-squares boundary matching. Because the diffracted fields have both TE and TM components, we need TE and TM vector modal functions to construct solutions. The vector modal functions are derived from the Floquet modes (separated solutions of scalar Helmholtz's equations satisfying the periodicity and the radiation condition) and are defined by

$$\varphi_{jm}^{\text{TE}}(\boldsymbol{P}) = \boldsymbol{e}_{jm}^{\text{TE}} \exp(j\boldsymbol{k}_{jm} \cdot \boldsymbol{P})$$
  
with  $\boldsymbol{e}_{jm}^{\text{TE}} = (\boldsymbol{k}_{jm} \times \boldsymbol{i}_z) / |\boldsymbol{k}_{jm} \times \boldsymbol{i}_z|,$  (7)

$$\varphi_{jm}^{\text{TM}}(\boldsymbol{P}) = \boldsymbol{e}_{jm}^{\text{TM}} \exp(j\boldsymbol{k}_{jm} \cdot \boldsymbol{P})$$
  
with  $\boldsymbol{e}_{jm}^{\text{TM}} = (\boldsymbol{e}_{jm}^{\text{TE}} \times \boldsymbol{k}_{jm}) / |\boldsymbol{e}_{jm}^{\text{TE}} \times \boldsymbol{k}_{jm}|,$   
 $m = 0, \pm 1, \pm 2, \dots \quad (\boldsymbol{P} \in V_j, j = 1, 2, 3).$  (8)

Here,  $i_z$  is a unit vector in the z direction and

are the wavevectors of the *m*th order space harmonics in  $V_i$  with

$$\alpha_m = \alpha + 2m\pi/d, \qquad (10)$$

and

$$\gamma_{jm}^{2} = (n_{j}\boldsymbol{k})^{2} - (\alpha_{m}^{2} + \beta^{2}), \operatorname{Re}(\gamma_{jm}) \ge 0, \operatorname{Im}(\gamma_{jm}) \ge 0.$$
(11)

Note that  $\varphi_{jm}^{\text{TE}}$  and  $\varphi_{jm}^{\text{TM}}$  modal functions will be employed in constructing approximations for the diffracted electric fields. For the magnetic fields we define

$$\psi_{jm}^{q}(\boldsymbol{P}) = (\omega \mu_{0})^{-1} \boldsymbol{k}_{jm} \times \varphi_{jm}^{q}(\boldsymbol{P}) \quad (q = \text{TE, TM; } j = 1, 2, 3),$$
(12)

which are obtained from  $\varphi_{jm}^q$  through Maxwell's equations. Note further that the modal functions in  $V_1$  are up-going plane waves while those in  $V_3$  are down-going. The modal functions in  $V_2$ , however, include both up- and down-going waves. To distinguish the travelling direction of a modal function in  $V_2$ , we use superscripts '+' and '-' representing up- and down-going waves.

We form approximations for the diffracted electric and magnetic fields in regions  $V_j$  (*j*=1, 2, 3) in terms of finite linear combinations of the TE and TM vector modal functions:

$$\begin{bmatrix} \boldsymbol{E}_{1N}^{d} \\ \boldsymbol{H}_{1N}^{d} \end{bmatrix} (\boldsymbol{P}) = \sum_{m=-N}^{N} A_{1m}^{\text{TE}}(N) \begin{bmatrix} \boldsymbol{\varphi}_{1m}^{\text{TE}} \\ \boldsymbol{\psi}_{1m}^{\text{TE}} \end{bmatrix} (\boldsymbol{P}) + \sum_{m=-N}^{N} A_{1m}^{\text{TM}}(N) \begin{bmatrix} \boldsymbol{\varphi}_{1m}^{\text{TM}} \\ \boldsymbol{\psi}_{1m}^{\text{TM}} \end{bmatrix} (\boldsymbol{P}),$$
(13)

$$\begin{bmatrix} \boldsymbol{E}_{2N}^{d} \\ \boldsymbol{H}_{2N}^{d} \end{bmatrix} (\boldsymbol{P}) = \sum_{m=-N}^{N} A_{2m}^{\text{TE+}}(N) \begin{bmatrix} \varphi_{2m}^{\text{TE+}} \\ \boldsymbol{\Psi}_{2m}^{\text{TE+}} \end{bmatrix} (\boldsymbol{P}) + \sum_{m=-N}^{N} A_{2m}^{\text{TM+}}(N) \begin{bmatrix} \varphi_{2m}^{\text{TM+}} \\ \boldsymbol{\Psi}_{2m}^{\text{TM+}} \end{bmatrix} (\boldsymbol{P}) + \sum_{m=-N}^{N} A_{2m}^{\text{TE-}}(N) \begin{bmatrix} \varphi_{2m}^{\text{TE-}} \\ \boldsymbol{\Psi}_{2m}^{\text{TE-}} \end{bmatrix} (\boldsymbol{P}) + \sum_{m=-N}^{N} A_{2m}^{\text{TM-}}(N) \begin{bmatrix} \varphi_{2m}^{\text{TM-}} \\ \boldsymbol{\Psi}_{2m}^{\text{TM-}} \end{bmatrix} (\boldsymbol{P}), \begin{bmatrix} \boldsymbol{E}_{3N}^{d} \\ \boldsymbol{H}_{3N}^{d} \end{bmatrix} (\boldsymbol{P}) = \sum_{m=-N}^{N} A_{3m}^{\text{TE}}(N) \begin{bmatrix} \varphi_{3m}^{\text{TE}} \\ \boldsymbol{\Psi}_{3m}^{\text{TM-}} \end{bmatrix} (\boldsymbol{P}) + \sum_{m=-N}^{N} A_{3m}^{\text{TM}}(N) \begin{bmatrix} \varphi_{3m}^{\text{TM}} \\ \boldsymbol{\Psi}_{3m}^{\text{TM}} \end{bmatrix} (\boldsymbol{P}),$$
(15)

here, N is a truncation size and the notation  $A_{jm}^q(N)$  (q=TE, TM) means that the  $A_{jm}^q$  coefficient depends on N.

Because the approximations above already satisfy the requirements (D1), (D2), and (D3), the modal coefficients should be determined in order that the approximations meet the boundary condition (D4). According to Yasuura's method, this boundary matching is done in the sense of least squares. That is, we look for the coefficients that minimize the meansquares boundary residual

$$I_{N} = \left\| \boldsymbol{v} \times (\boldsymbol{E}_{1N}^{d} + \boldsymbol{E}^{i} - \boldsymbol{E}_{2N}^{d}) \right\|_{S_{10}}^{2} + \left\| \boldsymbol{v} \times (\boldsymbol{E}_{2N}^{d} - \boldsymbol{E}_{3N}^{d}) \right\|_{S_{20}}^{2} + W^{2} \left\| \boldsymbol{v} \times (\boldsymbol{H}_{1N}^{d} + \boldsymbol{H}^{i} - \boldsymbol{H}_{2N}^{d}) \right\|_{S_{10}}^{2}$$
(16)  
$$+ W^{2} \left\| \boldsymbol{v} \times (\boldsymbol{H}_{2N}^{d} - \boldsymbol{H}_{3N}^{d}) \right\|_{S_{20}}^{2}.$$

Here,  $S_{10}$  and  $S_{20}$  denote the first period of the upper and the lower surface, v is a unit normal vector to the surfaces, W is a constant (the intrinsic impedance of vacuum is usually employed), and  $||f||_{S_{j0}}$  denotes a mean-square norm of a function f defined on  $S_{j0}$  (j=1, 2).

To solve this least-squares problem on a computer, we should discretize the problem to have a least-squares problem stated in a finite-dimensional vector space. This is done first by locating equallyspaced J sampling points on both  $S_{10}$  and  $S_{20}$ . Then, removing the common phase dependence  $e^{j\alpha x}$  and applying the trapezoidal rule, we have an approximation of  $I_N$  in the form that

$$I_{NJ} = \frac{d}{J} \left\| \boldsymbol{\Phi} \boldsymbol{A} - \boldsymbol{f} \right\|^2, \qquad (17)$$

here,  $\Phi$  is an  $8J \times 8(2N+1)$  Jacobian, A is an 8(2N+1)dimensional solution vector, and f is an 8J-dimensional vector whose lower 4J elements are zero. Although the derivation of Eq.(17) via Eq.(16) is closely related to Yasuura's theory (Yasuura and Itakura, 1965a; 1996a; 1966b; Yasuura, 1971), there is an alternative way that is straightforward. We introduce the second way in Appendix A for readers' convenience.

It is accepted knowledge that the number of sampling points in Yasuura's method should be J=2(2N+1) (Okuno, 1990). Hence, the size of the Jacobian is  $16(2N+1)\times8(2N+1)$ . We employ the singular-value decomposition (SVD) or the QR decomposition in solving the discretized least-squares problem above (Lawson and Hanson, 1974). Usually we prefer the QR algorithm because it is faster than the SVD algorithm. We apply the SVD when we need to examine the nature of the least-squares problem for some purpose, e.g., in finding a necessary and sufficient number of sampling points or in looking for an appropriate location of the sampling points.

## NUMERICAL RESULTS

Here we show some numerical results obtained by the method described in the preceding section. After making necessary preparation, we show the results for both the planer-mounting and conical-mounting cases.

# Preparation

The grating is assumed to be made of silver and the period and the depth are given by  $d=0.556 \ \mu\text{m}$  and  $2h=0.006 \ \mu\text{m}$ . The thickness to period ratio e/d is a parameter varying from 0.02 ( $e=0.01112 \ \mu\text{m}$ ) to 0.4 ( $e=0.2224 \ \mu\text{m}$ ). As an incident light we choose a monochromatic plane wave whose wavelength is  $\lambda=0.650 \ \mu\text{m}$ . The refractive index of silver at this wavelength is given by  $n_2=0.07+4.20$ j (Hass and Hadley, 1963). It should be noted, however, that the index of a metal film depends not only on the wavelength but also on the thickness of the film, in particular when the film is extremely thin. It may take unusual values if circumstances require. When dealing with a thin metal structure, hence, we should be careful in using the index value given in the literature. As for the value taken in our computation, we assume that  $n_2=0.07+4.20j$  is available even for the case of e/d=0.02 ( $e=0.2224 \mu m$ ). This is because a similar assumption was supported by experimental data in a problem of diffraction by an aluminum grating with a thin gold over-coating.

The resonance absorption is observed primarily as a dip of an efficiency curve. The *m*th order TE- and TM-wave efficiency are defined for the propagating orders in regions  $V_1$  and  $V_3$  as

$$\rho_{jm}^{q} = (\gamma_{jm} / \gamma) |A_{jm}^{q}|^{2} \quad (q=\text{TE, TM}; j=1, 3). \quad (18)$$

The efficiency of an *m*th order propagating mode is given by

$$\rho_{jm} = \rho_{jm}^{\text{TE}} + \rho_{jm}^{\text{TM}} \quad (j=1, 3),$$
(19)

and a total efficiency

$$\rho^{\text{total}} = \sum_{j,m} \rho_{jm} \tag{20}$$

is a sum of the efficiency of all the propagating orders. It is worth mentioning that the efficiency of a propagating mode is per period power carried away by the propagating mode normalized by the incident power. The quantity  $1-\rho^{\text{total}}$ , hence, is the extinction power absorbed in the grating provided the  $A_{jm}^q$  coefficients are accurate. Because convergence of solutions has been proven in Yasuura's method, we can employ the  $A_{jm}^q(N)$  coefficients with a sufficiently large N in evaluating the absorbed power, the large N for which the coefficients are stable.

#### **Planer-mounting case**

Here we examine the resonance absorption from a couple of viewpoints: diffraction efficiency, behavior of modal coefficients, field distribution, and power flow. Because there is no mode conversion in planer mounting, we deal with the TM-wave (p-polarization) incidence alone in this subsection.

1. Diffraction efficiency

Fig.3 shows the total diffraction efficiency of a thin silver grating as functions of the angle of incidence. We observe partial absorption of incident light as the dips of efficiency curves in addition to the constant absorption corresponding to the reflectivity of silver. We assume that the dips are caused by the excitation of surface plasmons. If this is the case, each of the dips is related to one of the three types of plasmon modes: a single-interface surface plasmon (SISP) that is observed as the single dip at  $\theta$ =7.95° on the e/d=0.4 curve; a short-range surface plasmon (SRSP) seen at  $\theta$ =6.41° on e/d=0.08 curve and at  $\theta$ =18.30° on e/d=0.02 curve; and a long-range surface plasmon (LRSP) found at  $\theta$ =8.78° on e/d=0.08 and  $\theta$ =9.63° on e/d=0.02.



Fig.3 Total diffraction efficiency  $\rho^{\text{total}}$  as functions of the angle of incidence  $\theta$ 

Figs.4a and 4b show the normalized power carried away by the zeroth order reflected (in  $V_1$ ) and transmitted (in  $V_3$ ) mode. When the grating is thick (e/d=0.4), the power can be seen in  $V_1$  alone and no transmitted power exists in  $V_3$ . Increasing  $\theta$  from 0°, we first observe the dip at  $\theta=7.95^\circ$  corresponding to the absorption in Fig.3. Increasing  $\theta$  further, we meet a small anomaly at  $\theta=9.63^\circ$  at which the -1 order starts propagating to carry the difference of power between Fig.3 and Fig.4a. While if the grating is relatively thin (e/d=0.08), the power exists in both  $V_1$ and  $V_3$ . Although the power in  $V_3$  is small in general, it becomes large at the angles of incidence at which the absorption is observed in Fig.3. This suggests that coupled oscillations occur on the upper and lower surface of the grating. When the grating is extremely thin (e/d=0.02), which is comparable to the skin depth of silver at this wavelength, the grating is almost transparent and the power in  $V_3$  is nearly the same as that in  $V_1$ . The result of coupled oscillations can be seen clearly at  $\theta=9.63^\circ$ , which corresponds to the LRSP as we will see later. While the oscillations at  $\theta=18.30^\circ$ , which are related to the SRSP, are not so evident. This difference comes mainly from the even and odd nature of the LRSP and SRSP.



Fig.4 Zeroth order diffraction efficencies  $\rho_{1,0}^{\text{TM}}$  (a) and  $\rho_{3,0}^{\text{TM}}$  (b) as functions of  $\theta$ 

2. Expansion coefficients

We examine the same phenomena observing the modal coefficients in  $V_j$  (*j*=1, 3). Figs.5 and 6 illustrate the -1 order modal coefficients  $A_{jm}^{\text{TM}}$  for e/d=0.4 and 0.08. Fig.7, in addition to the -1 order, shows the +1 order coefficients for e/d=0.02. This is because the

order of the evanescent mode that couples the surface plasmons is -1 in the cases of e/d=0.4 and 0.08 and is  $\pm 1$  in the e/d=0.02 case.

We observe in Fig.5a (e/d=0.4) resonance character of the coefficient  $A_{1,-1}^{TM}$  near  $\theta=7.95^{\circ}$ : enhancement and rapid change in phase. While the coefficient  $A_{3,-1}^{TM}=0$  remains unchanged as we see in Fig.5b. This means that the incident light causes a coupling between the -1 order evanescent mode and an oscillation on the upper surface of the grating. The oscillation exists locally in the vicinity of the illuminated surface and, hence, does not have any influence on the field in  $V_3$ . We will see later that the substance of the oscillation is the plasmon surface wave using a phase-matching condition. The specific angle at which the absorption occurs will be called a resonance angle hereafter. In Fig.6 (e/d=0.08) we find the resonance features in both  $A_{1,-1}^{\text{TM}}$  and  $A_{3,-1}^{\text{TM}}$ . They, in addition, appear around two angles of incidence:  $\theta=6.5^{\circ}$  and  $8.8^{\circ}$ . This means that the oscillation in the vicinity of the lit surface causes another oscillation on the lower surface at this thickness. The oscillations interfere with each other and result in two coupled modes: the SRSP and LRSP. Because the eigenvalues of the coupled modes are different from each other, we observed two dips in Fig.3 at the resonance angles corresponding to the eigenvalues. We will show later a method for predicting the resonance angles.

In Fig.7 (e/d=0.02) we observe similar resonance characteristics of  $A_{1,-1}^{TM}$  and  $A_{3,-1}^{TM}$  at  $\theta=9.63^{\circ}$ , which corresponds to the sharp dip in Fig.3. At this resonance angle the -1 order evanescent mode couples the oscillations to excite an LRSP mode. While at  $\theta=18.3^{\circ}$ 





Fig.5 The -1 order modal coefficients  $A_{1,-1}^{\text{TM}}$  (a) and  $A_{3,-1}^{\text{TM}}$  (b) as functions of  $\theta$  at e/d=0.4

Fig.6 The -1 order modal coefficients  $A_{l,-1}^{\text{TM}}$  (a) and  $A_{3,-1}^{\text{TM}}$  (b) as functions of  $\theta$  at e/d=0.08

where the broad dip occurred in Fig.3, no distinct feature can be seen in  $A_{1,-1}^{\text{TM}}$  or  $A_{3,-1}^{\text{TM}}$ . Instead we notice weak resonance in  $A_{1,1}^{\text{TM}}$  and  $A_{3,1}^{\text{TM}}$  at this resonance angle. Here, the +1 order evanescent mode couples the oscillations to excite an SRSP mode.



Fig.7 Modal coefficients  $A_{1,-1}^{\text{TM}}$  and  $A_{1,1}^{\text{TM}}$  (a);  $A_{3,-1}^{\text{TM}}$  and  $A_{3,1}^{\text{TM}}$  (b) as functions of  $\theta$  at e/d=0.02

# 3. Field distribution and energy flow

We consider the same phenomena observing field distribution and energy flow near the grating surfaces. In the former we find that the total field is enhanced and that the -1 or +1 diffraction order is dominant at the resonance angle. In the latter we observe the symmetric (even) and anti-symmetric (odd) nature of the oscillations, which correspond to the LRSP and SRSP.

Figs.8~12 show the field distribution (a) and energy flow (b) in the vicinity of the grating surface at

the resonance angles observed in Fig.3. Although the parameters in these figures are the same as before, we show the relative thickness e/d and the resonance angles in Table 1 for readers' convenience. The table, in addition, includes the number of the evanescent mode that couples the oscillations and the possible type of the plasmon mode.

To draw the field distribution we first calculate

Table 1 Thickness, angle of incidence, number of eva-nescent order, and type of plasmon\*

Fig.	e/d	$\theta$ (degree)	Mode	Туре
8	0.40	7.95	-1	SISP
9	0.08	6.41	-1	SRSP
10	0.08	8.78	-1	LRSP
11	0.02	9.63	-1	LRSP
12	0.02	18.30	+1	SRSP

\**h*=0.03 μm, *d*=0.556 μm, *λ*=0.650 μm



Fig.8 Field distribution ( $|E^t|$  and  $|E_{j,-1}^{TM}|$ ) (a) and energy flow (b) at  $\theta$ =7.95°, which corresponds to the single dip on the *e*=0.4 curve in Fig.3

the total field  $E^{t} = E^{i} + E_{j}^{d}$  and the electric field of -1 (or +1) order diffracted mode  $E_{jm}^{TM} = A_{jm}^{TM} \varphi_{jm}^{TM}$  (*m*=-1 or 1) in each region. Then, taking the absolute values, we plot the distribution shown in Figs.8a, 9a, 10a, 11a, 12a. The abscissa and ordinate show the field magnitude and a normalized distance in *z*. The parallel broken lines are the grating surfaces.

The energy flow at a point P is given by Re[S(P)], where  $S(P)=(1/2)E^{t}(P)\times \overline{H^{t}(P)}$  stands for Poynting's vector,  $E^{t}$  and  $H^{t}$  denote total fields, and the over-bar means complex conjugate. We calculate the energy flow at each point located densely near the grating surface and show the results in Figs.8b, 9b, 10b, 11b, 12b.

Now let us examine the results in each figure. Fig.8a shows the field distribution (total and -1 order) for the thick case (e/d=0.4) at  $\theta=7.95^{\circ}$ , which corresponds to the single dip in Fig.3. In this figure we

 $|E^{i}+E^{d}|$ 

0.5

0.4

SRSP

notice strong enhancement of the total electric field (Note that the magnitude of the incident radiation is 1), the enhancement which is observed only in the vicinity of the resonance angles. The total field above the grating surface decays exponentially in z and the configuration and the magnitude are almost the same as those of the -1 order evanescent mode. The state of affairs is nearly the same in the metal region except for the rapid decay. Because the grating is thick, the oscillation near the upper surface does not reach the lower surface and, hence, the field below the grating is zero. Fig.8b illustrates the energy flow S, which is magnified by 25 in the metal region. We see that the energy flow is almost in the x direction and that it goes in opposite directions in vacuum and in metal. This is commonly observed when an SISP is excited.

Figs.9 and 10 show the same thing for the relatively thin case (e/d=0.08). Fig.9 illustrates the results at  $\theta=6.41^{\circ}$  where the left dip is observed in Fig.3.





Fig.9 Field distribution ( $|E^t|$  and  $|E_{j,-1}^{TM}|$ ) (a) and energy flow (b) at  $\theta$ =6.41°, which corresponds to the left dip on the *e*=0.08 curve in Fig.3

Fig.10 Field distribution ( $|E^t|$  and  $|E_{j,-1}^{TM}|$ ) (a) and energy flow (b) at  $\theta$ =8.78°, which corresponds to the right dip on the *e*=0.08 curve in Fig.3

While Fig.10 depicts the results at  $\theta$ =8.78°, the right dip in Fig.3. In Figs.9a and 10a we notice again the enhancement of the total filed and the dominating nature of the -1 order evanescent mode. The rate of enhancement in Fig.9a is not so large as that in Fig.10a. We can understand the difference assuming that the former and the latter are the results of the LRSP and the SRSP mode excitation. Figs.9b and 10b complement the understanding showing the even and odd nature of relevant oscillations.

Figs.11 and 12 are the results for the extremely thin case (e/d=0.02). We can repeat similar discussions except that the +1 order evanescent mode couples with the oscillation in Fig.12 and that strong enhancement (Fig.11) and cancellation (Fig.12) are seen as the results of an extremely thin metal structure.

4. Prediction of resonance angles

As we suggested before, the resonance absorption occurs at a specific angle of incidence (the resonance angle) at which the *x*-direction phase constant of an evanescent order agrees with the real part of an eigenvalue of a plasmon mode on a metal grating. Hence, if we find the eigenvalue, we can predict the resonance angle. A method for finding the eigenvalue (propagation constant) was proposed by Neviere (1980), who evaluated the propagation constant of a surface plasmon mode as a complex pole of a scattering matrix for the diffraction problem. We here provide an alternative algorithm that is efficient in numerical computations: Instead of finding the poles of the scattering matrix, we look for a complex-valued angle of incidence at which  $|A_{lm}^{TM}|$  takes a maximal value. Here, *m* is a diffraction order that is assumed to couple the surface plasmons.

To find the angle of incidence we first calculate the propagation constant  $\alpha_{\text{flat}}$  of a plasmon mode (SISP, SRSP, or LRSP) that can be excited on a plane





Fig.11 Field distribution ( $|E^t|$  and  $|E_{j,-1}^{\text{TM}}|$ ) (a) and energy flow (b) at  $\theta$ =9.63°, which corresponds to the left dip on the *e*=0.02 curve in Fig.3

Fig.12 Field distribution ( $|E^t|$  and  $|E_{j,1}^{\text{TM}}|$ ) (a) and energy flow (b) at  $\theta$ =18.3°, which corresponds to the left dip on the *e*=0.02 curve in Fig.3

interface. Then, we set

$$\sin\theta_{\rm init} + m\lambda / d = \hat{\alpha}_{\rm flat} = \alpha_{\rm flat} / k \tag{21}$$

to have an initial guess  $\theta_{init}$  in an iteration procedure for finding the complex-valued angle of incidence  $\theta_{sp}$ that makes  $|A_{lm}^{TM}|$  maximum. In the iteration we solve diffraction problems with complex incident angles by using Yasuura's method and seek  $\theta_{sp}$  employing a quasi-Newton algorithm. On having the  $\theta_{sp}$ , we obtain a normalized propagation constant expressed by

$$\hat{\alpha}_{\rm sp} = \sin \theta_{\rm sp} + m\lambda/d. \tag{22}$$

We can predict the resonance angle  $\theta_r$  by using a phase-matching condition

$$\operatorname{Re}\hat{\alpha}_{\rm sp} = \sin\theta_{\rm r} + m\lambda/d \tag{23}$$

and by solving this equation with respect to  $\theta_{\rm r}$ .

Table 2 shows the propagation constant  $\hat{\alpha}_{sp}$ 

obtained through the iteration procedure, the predicted resonance angle  $\theta_r$ , and the angle of incidence  $\theta_d$  at which the absorption occurred in Fig.3. The good agreement between  $\theta_r$  and  $\theta_d$  supports our assumption in subsection "Diffraction efficiency".

5. Thickness dependence of  $\hat{\alpha}_{sp}$ 

In Fig.13 we show the normalized propagation constant  $\hat{\alpha}_{sp}$ , as a function of the thickness e/d. It is seen clearly that the SISP alone is excited for a relatively thick grating  $(e/d \ge 0.2)$  and that  $\hat{\alpha}_{sp}$  is almost independent of e/d in that range of thickness. When e/d decreases from 0.2, the curve splits into two that correspond to the SRSP and LRSP. The nature of  $\hat{\alpha}_{sp}$  for the SRSP ( $\hat{\alpha}_{SRSP}$ ) and that for the LRSP ( $\hat{\alpha}_{LRSP}$ ) are considerably different:

(C1)  $|\hat{\alpha}_{\text{SRSP}}|$  depends strongly on e/d and increases with decrease of e/d; while  $|\hat{\alpha}_{\text{LRSP}}|$  decreases slightly.

(C2)  $\hat{\alpha}_{\text{SRSP}}$  has a relatively large imaginary part that increases with decrease of e/d; whereas the



Fig.13 Real part (a) and imaginary part (b) of  $\hat{a}_{sp}$  as a function of e/d

Table 2 Propagation constants of plasmon modes, predicted resonance angles, and the angles at which absorption occurred $^*$ 

e/d	Mode	Туре	${ m Re}\hat{lpha}_{ m sp}$	$\mathrm{Im}\hat{\alpha}_{\mathrm{sp}}$	$\theta_{\rm r}$ (degree)	$\theta_{\rm d}$ (degree)
0.40	-1	SISP	-1.03069769	-0.003400046	8.00	7.95
0.08	-1	SRSP	-1.05735615	-0.006013251	6.47	6.41
0.08	-1	LRSP	-1.01633632	-0.001975368	8.84	8.78
0.02	+1	SRSP	-1.48586084	-0.028050984	18.47	18.30
0.02	-1	LRSP	-1.00184339	-0.000331986	9.63	9.63

\* *h*=0.03 μm, *d*=0.556 μm, *λ*=0.650 μm

imaginary part of  $\hat{\alpha}_{LRSP}$  is small and approaches zero.

Because of (C1), the resonance angles of LRSP and SRSP, respectively, are in close vicinity to and apart from that of the SISP. Item (C2) means that the resonance is stronger in the LRSP than in the SRSP. In addition, the resonance in the SISP becomes weak when e/d is reduced. These properties estimated from the thickness dependence of  $\hat{\alpha}_{sp}$  are in good agreement with the results shown in subsections from "Diffraction

efficiency" to "Field distribution and energy follow".

#### **Conical-mounting case**

Here, we show some results obtained in the conical mounting case in which the azimuth angle  $\phi=30^{\circ}$  is fixed. In that case, the resonance absorption occurs not only for the TM-wave incidence but also for the TE-wave incidence (Matsuda *et al.*, 1999; Bryan-Brown *et al.*, 1990). Let us assume, for simplicity, a TE-wave is incident on the grating placed in conical mounting. Then the diffracted waves consist of both TE- and TM-components because TE-components alone cannot satisfy the boundary conditions. Hence, the conical mounting necessarily causes TE-TM mode conversion, and the TM component of an evanescent diffraction odder can couple the surface plasmons.

Fig.14 shows the total diffraction efficiency as a function of  $\theta$  for several e/d's (e/d=0.4, 0.08, 0.02). In the efficiency curves we observe partial absorption of incident light as the dips that occur at the same angles for both TE- and TM-wave incidence. Comparing them with the figures in the planar mounting case, we find that each curve shows much the same behavior as that in the planar mounting, just with a slight shift in the location of dips. Each one of the dips in Fig.14a relates to one of the three types of plasmon modes. The SISP is observed as the single dip at  $\theta$ =9.40° on the e/d=0.4 curve; the SRSP is found at  $\theta=7.54^{\circ}$  on the e/d=0.08 curve and  $\theta=20.50^{\circ}$  on the e/d=0.02curve; and the LRSP is seen at  $\theta$ =11.47° on the e/d=0.08 curve and  $\theta=20.88^{\circ}$  on the e/d=0.02 curve. Classification of the dips into the three plasmon types can be done again by observing the field profile and energy flow shown below. In Fig.14b we observe almost the same behavior. Absorption peaks occur almost at the same angle of incidence: 9.42° (SISP); 7.56° and 20.88° (SRSP); 10.43° and 11.47° (LRSP).



Fig.14 Total diffraction efficiency  $\rho^{\text{total}}$  as a function of the angle of incidence  $\theta$  in conial mounting. (a) TM-wave incidence; (b) TE-wave incidence

Fig.15 illustrates the normalized power carried away by the zeroth order diffracted mode for a TM-wave incidence ( $\delta$ =90°). Figs.15a and 15b, respectively, correspond to the reflected and transmitted power.

In Figs.16, 17 and 18 we show the  $\theta$  dependence of the coefficients of evanescent space harmonics that couple the plasmon modes. As in the planar mounting case, we observe strong resonance character of the coefficients.

In Figs.19~23 we show the field distribution and energy flow in the vicinity of the grating surface at the angles of incidence at which the absorption was observed in Fig.14. From which, we can classify the dips into the three plasmon types. For readers' convenience, we show the values of resonance angle  $\theta$  as well as the plasmon type on the figures.



Fig.15 Zeroth order diffraction efficiencies  $\rho_{1,0}^{TM}$  (a) and  $\rho_{3,0}^{TM}$  (b) as functions of  $\theta$  in conial mounting



Fig.16 The -1 order modal coefficients  $A_{1,-1}^{TM}$  (a) and  $A_{3,-1}^{TM}$  (b) as functions of  $\theta$  at e/d=0.4



Fig.17 Modal coefficients  $A_{l,-1}^{\text{TM}}$  and  $A_{l,1}^{\text{TM}}$  (a);  $A_{3,-1}^{\text{TM}}$  and  $A_{3,1}^{\text{TM}}$  (b) as functions of  $\theta$  at e/d=0.08



Fig.18 Modal coefficients  $A_{1,-1}^{\text{TM}}$  and  $A_{1,1}^{\text{TM}}$  (a);  $A_{3,-1}^{\text{TM}}$  and  $A_{3,1}^{\text{TM}}$  (b) as functions of  $\theta$  at e/d=0.02



Fig.19 Field distribution ( $|E^{t}|$  and  $|E_{j,-1}^{TM}|$ ) (a) and energy flow (b) at  $\theta$ =9.40°, which corresponds to the single dip on the e=0.40 curve in Fig.14a



Fig.20 Field distribution ( $|E^t|$  and  $|E_{j,-1}^{TM}|$ ) (a) and energy flow (b) at  $\theta$ =7.54°, which corresponds to the left dip on the e=0.08 curve in Fig.14a



Fig.21 Field distribution ( $|E^t|$  and  $|E_{j,-1}^{TM}|$ ) (a) and energy flow (b) at  $\theta$ =10.42°, which corresponds to the right dip on the *e*=0.08 curve in Fig.14a



Fig.22 Field distribution ( $|E^t|$  and  $|E_{j,-1}^{TM}|$ ) (a) and energy flow (b) at  $\theta$ =11.47°, which corresponds to the left dip on the *e*=0.02 curve in Fig.14a



Fig.23 Field distribution ( $|E^t|$  and  $|E_{j,1}^{TM}|$ ) (a) and energy flow (b) at  $\theta$ =20.50°, which corresponds to the left dip on the *e*=0.02 curve in Fig.14a

### CONCLUSION

We solved the problem of plasmon resonance absorption in a thin metal grating placed in planer and conical mounting. Calculating diffraction efficiency, expansion coefficients, field profiles, and energy flow, we examined the characteristics of the absorption in detail. We showed that a plasmon surface wave is excited by coupling of an evanescent space harmonic with the surface wave and that the plasmons on a thin grating can be classified into one of the three types of plasmon modes: the SISP, SRSP, and LRSP. We gave an interpretation of the distinctive features of the three modes based on the even and odd nature of the modes and on the thickness dependence of plasmon wavenumbers.

We are working with detailed examination of the absorption in conical mounting, in which the azimuth angle has a large influence on the location and strength of the absorption and an enhanced TE-TM mode conversion occurs. This would be useful in practical application and is an important subject for further examination.

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### APPENDIX A: ALTERNATIVE WAY OF OBTAINING THE LEAST-SQUARES PROBLEM

It is worth to mention that Eq.(19) can be found alternatively first by describing the boundary conditions at each of the sampling points to obtain a set of linear equations with respect to the modal coefficients. Then, determining the number of sampling points in order that the number of linear equations be twice the number of unknowns (total number of  $\varphi_{jm}^q$  modal functions employed), we have an overdetermined set of linear equations. Requiring a least-squares solution of the set of equations, we have a least-squares problem with respect to a mean-square error given by Eq.(19). If we take this way, we first should notice that a sampling point provides us with four linear equations. This is because the tangential components of both electric and magnetic field should be continuous and a tangential component is described by two parameters, e.g., *x*- and *y*-component. Hence, if we locate *J* sampling points on both  $S_1$  and  $S_2$ , we have 8*J* linear equations with respect to the modal coefficients. On the other hand, because the number of unknowns is 8(2N+1), the required number of linear equations is 16(2N+1). This gives a recommended number of sampling points J=2(2N+1).